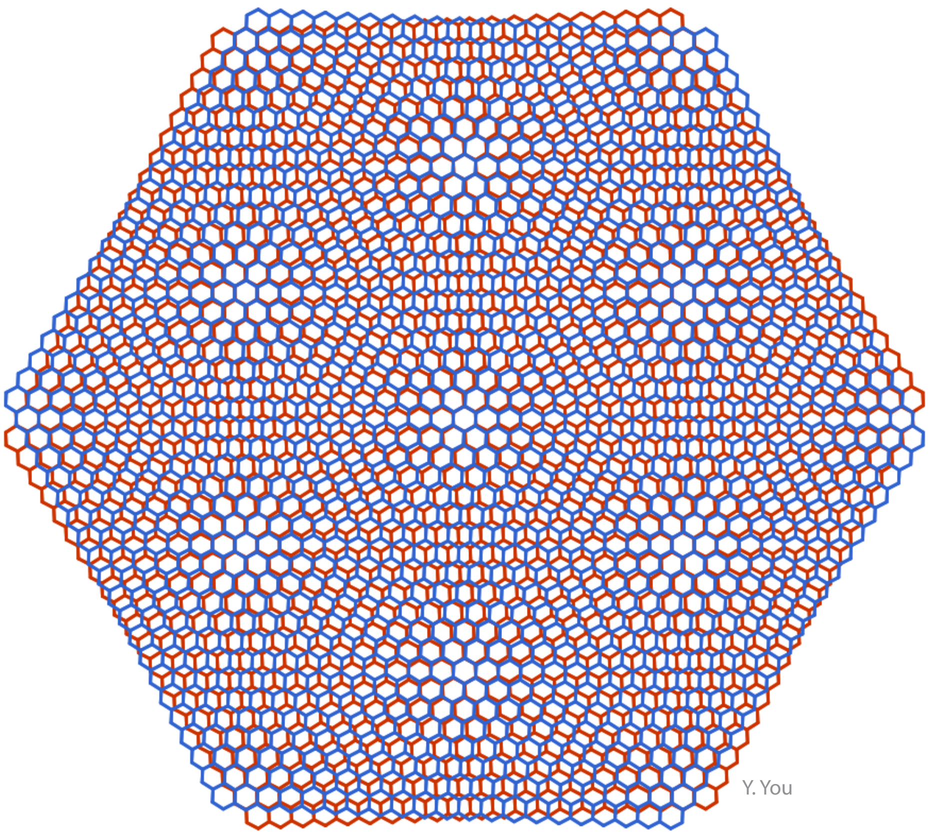
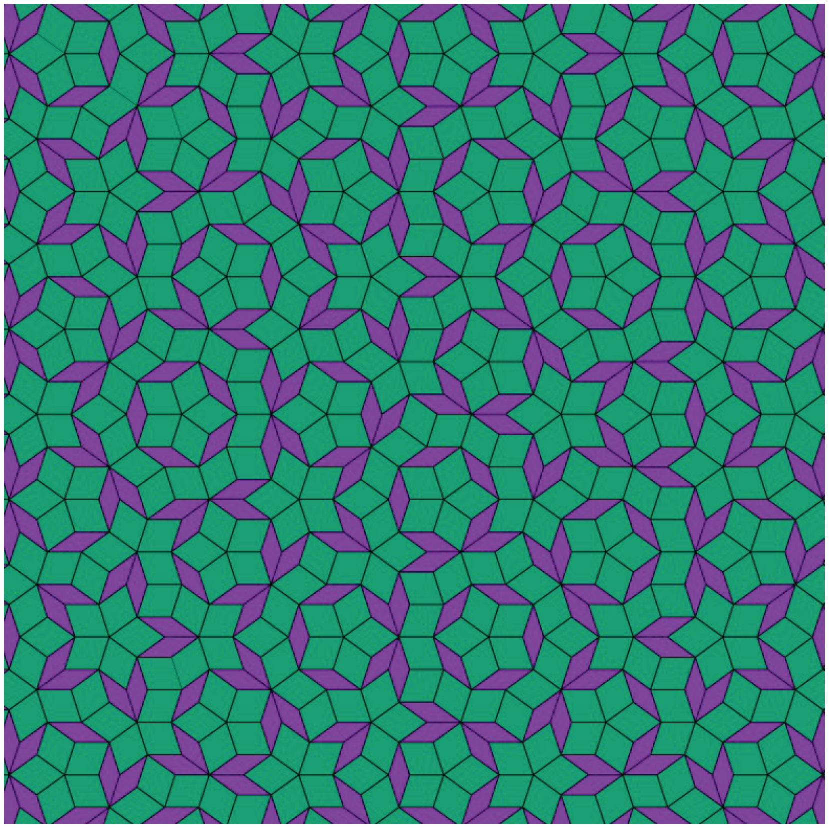
Twistronics, Quasicrystals, and Exotic Composite Materials

Kenneth M. Golden
Department of Mathematics
University of Utah



Moiré superlattice
twisted bilayer graphene



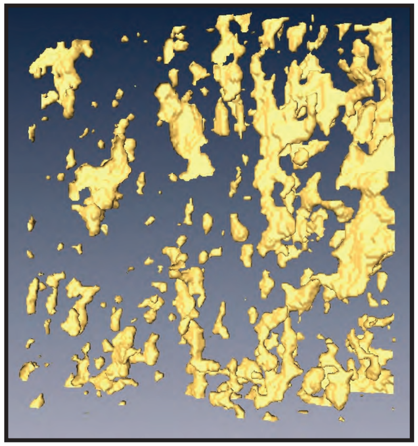
quasiperiodic Penrose tiling

Sea Ice is a Multiscale Composite Material

microscale

brine inclusions

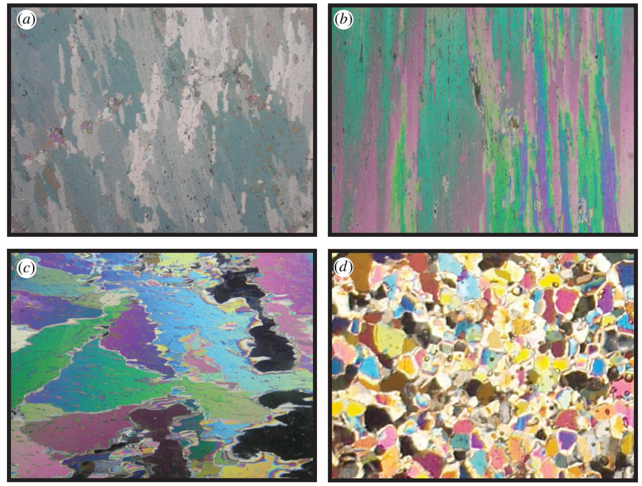
Weeks & Assur 1969



H. Eicken

Golden *et al. GRL* 2007

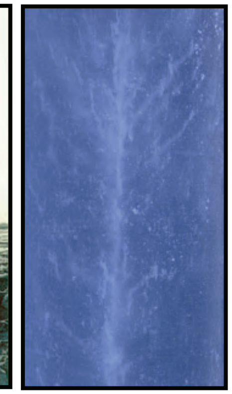
polycrystals



Gully *et al. Proc. Roy. Soc. A* 2015

brine channels

D. Cole



K. Golden

millimeters **centimeters**

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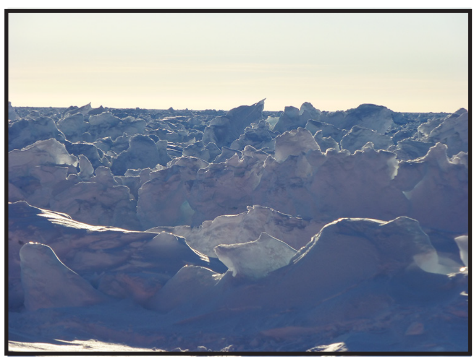
mesoscale

Arctic melt ponds

K. Frey

Antarctic pressure ridges



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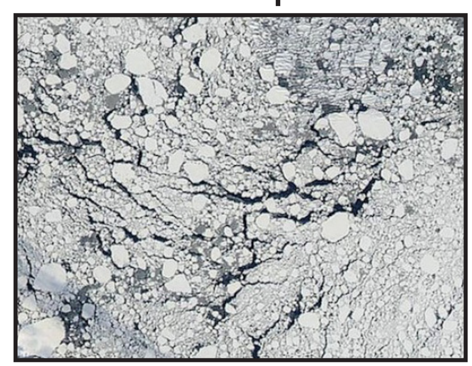
meters

macroscale

sea ice floes

J. Weller

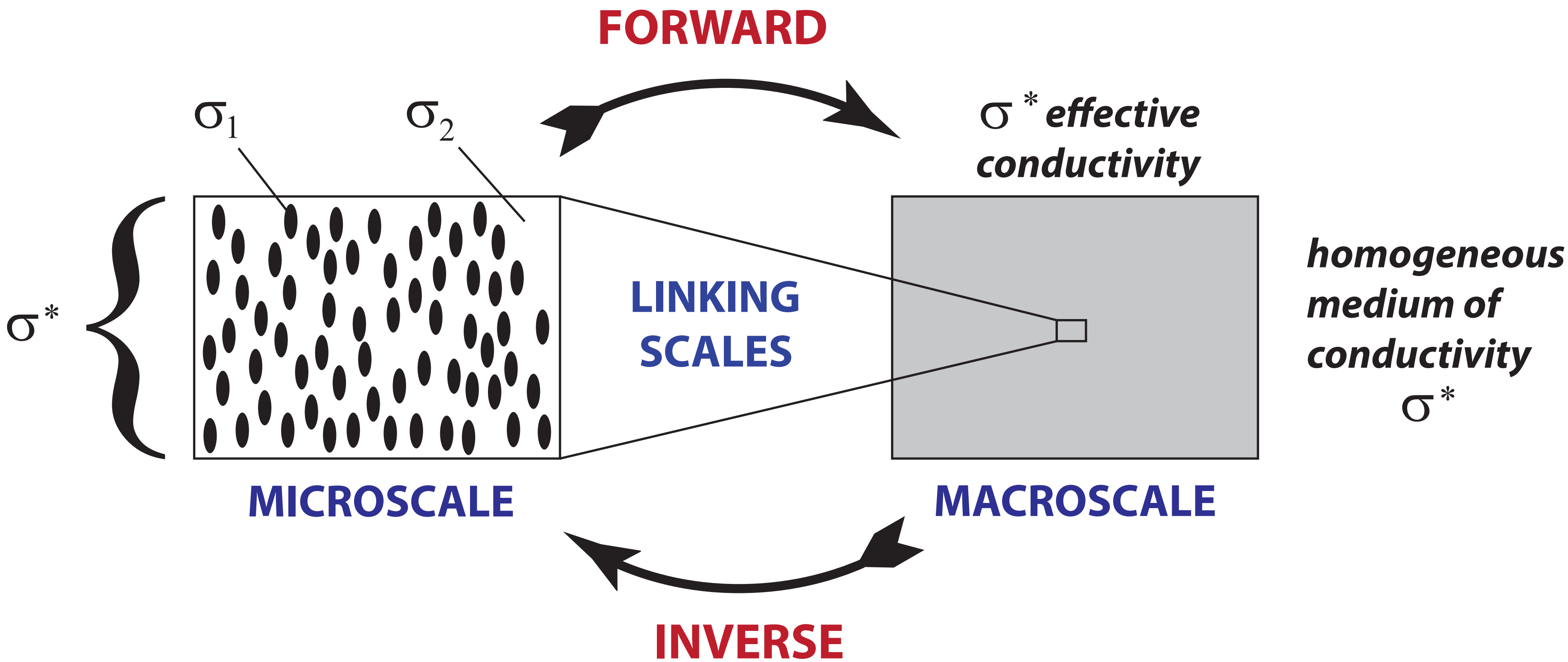
sea ice pack



NASA

kilometers

HOMOGENIZATION for Composite Materials

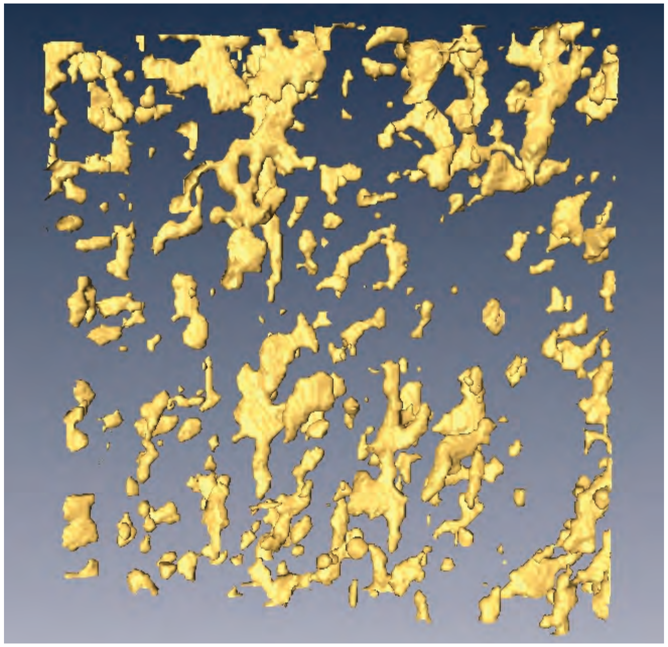


Maxwell 1873 : effective conductivity of a dilute suspension of spheres
Einstein 1906 : effective viscosity of a dilute suspension of rigid spheres in a fluid

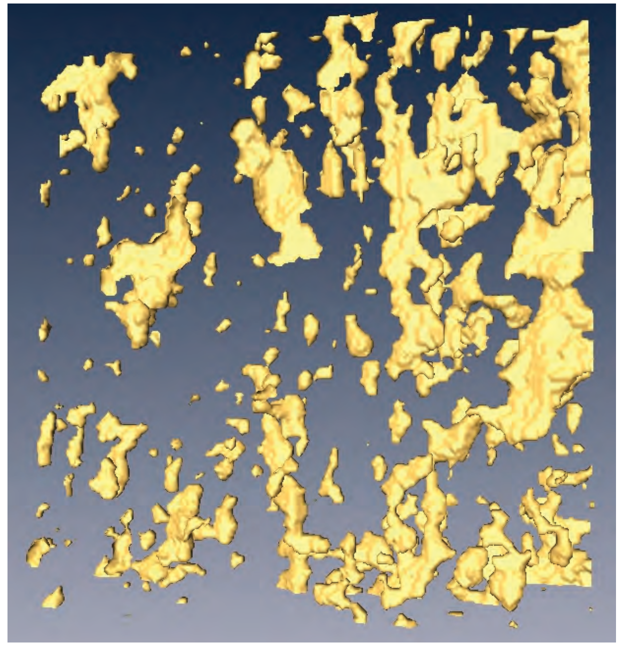
*Wiener 1912 : arithmetic and harmonic mean **bounds** on effective conductivity*
*Hashin and Shtrikman 1962 : variational **bounds** on effective conductivity*

widespread use of composites in late 20th century due in large part to advances in mathematically predicting their effective properties

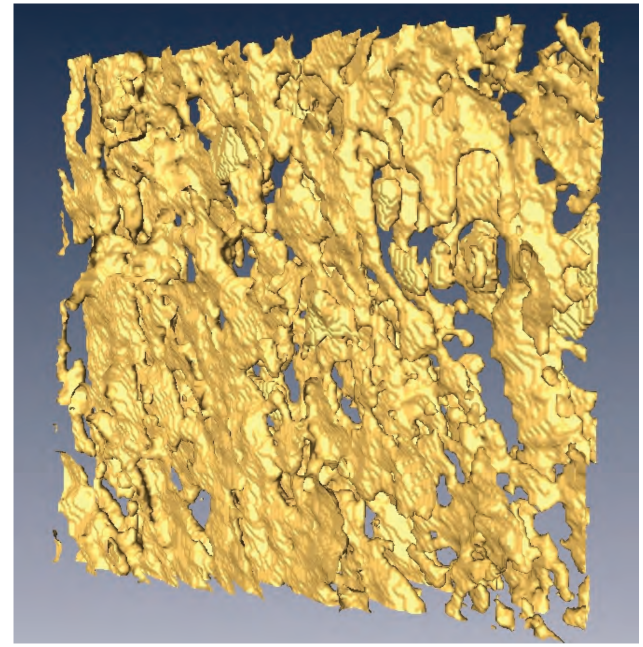
brine volume fraction and ***connectivity*** increase with temperature



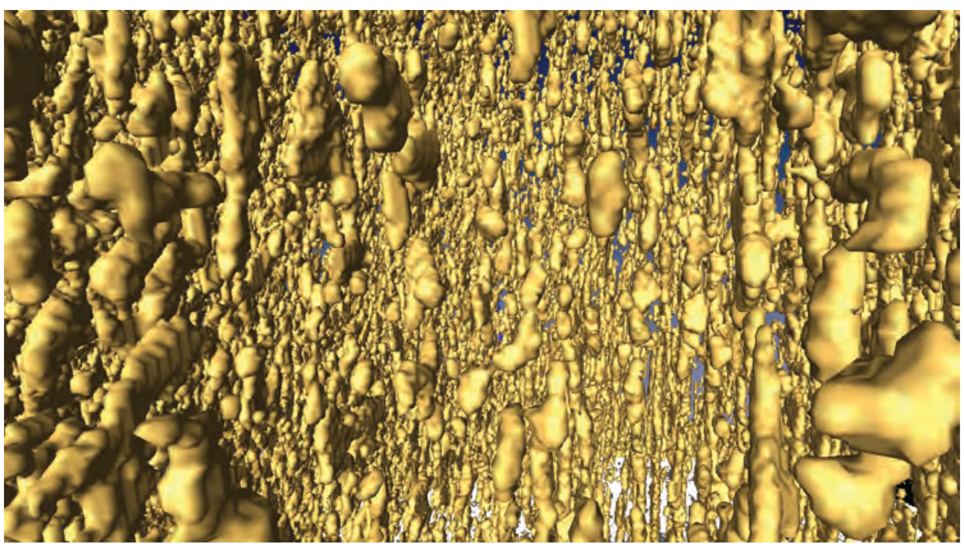
T = -15 °C, $\phi = 0.033$



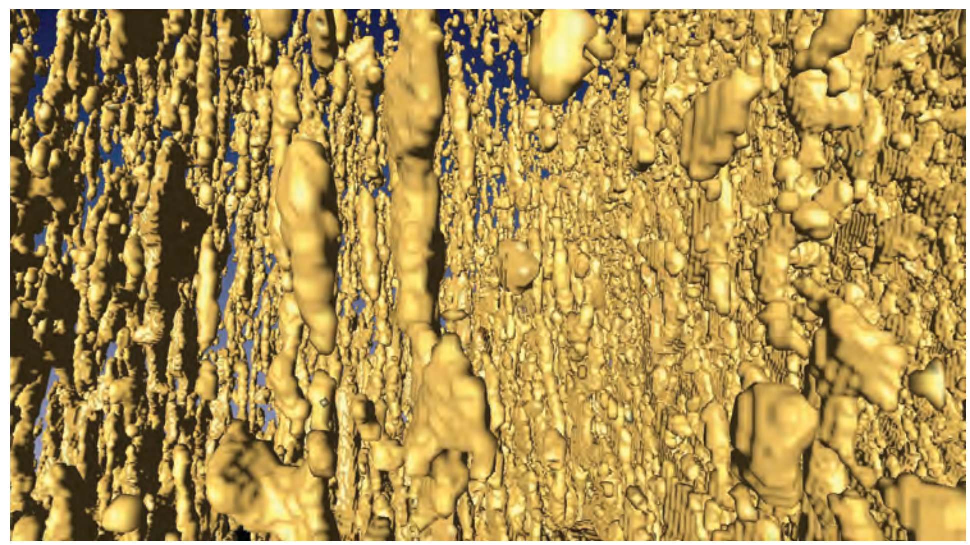
T = -6 °C, $\phi = 0.075$



T = -3 °C, $\phi = 0.143$



T = -8 °C, $\phi = 0.057$



T = -4 °C, $\phi = 0.113$

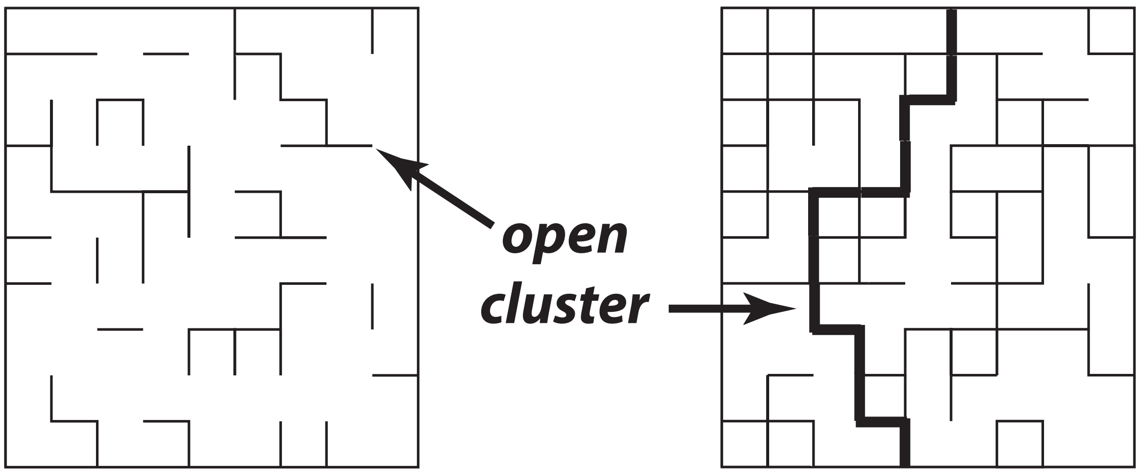
X-ray tomography for brine in sea ice

Golden *et al.*, *Geophysical Research Letters*, 2007

percolation theory

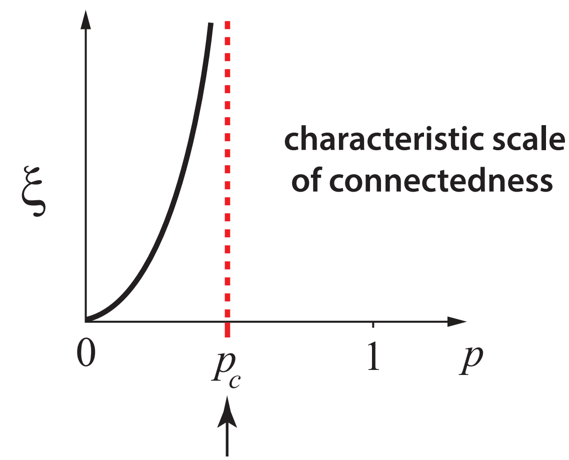
probabilistic theory of connectedness

impermeable | **permeable** | **correlation length**



$p = 1/3$ $\qquad$ $p = 2/3$

development of long range order



percolation threshold

bond → ***open*** *with probability* p
closed *with probability 1-p*

$$\xi(p) \sim |p - p_c|^{-\nu} \qquad p \rightarrow p_c$$

ν **universal: depends only on *d***

p_c depends on type of lattice and *d*

percolation threshold

$$p_c = 1/2 \quad \textbf{for} \quad \mathbf{d = 2}$$

smallest *p* for which there is an infinite open cluster

Remote sensing of sea ice

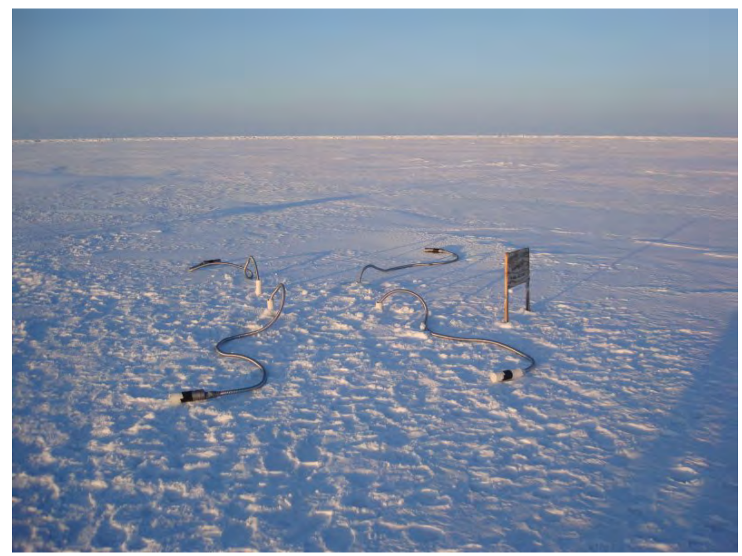
sea ice thickness
ice concentration

INVERSE PROBLEM

Recover sea ice properties from electromagnetic (EM) data

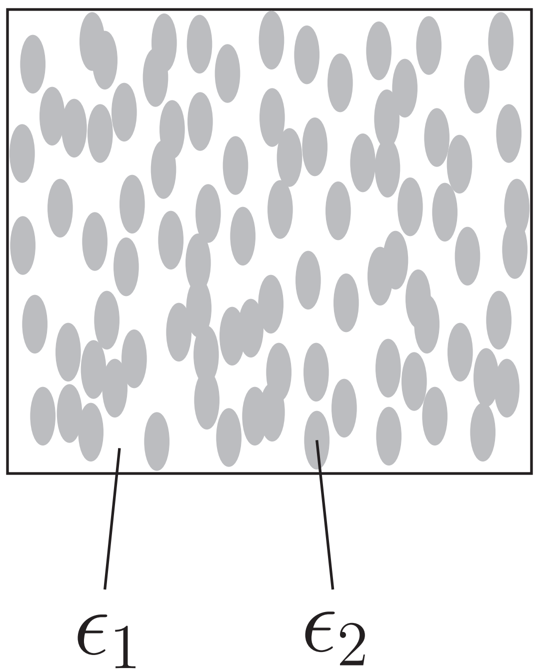
$$\varepsilon^*$$

effective complex permittivity
(dielectric constant, conductivity)



brine volume fraction
brine inclusion connectivity

Effective complex permittivity of a two phase composite in the quasistatic (long wavelength) limit



$$\epsilon^*$$

$$D = \epsilon E$$

$$\nabla \cdot D = 0$$

$$\nabla \times E = 0$$

$$\langle D \rangle = \epsilon^* \langle E \rangle$$

p_1 , p_2 = volume fractions of the components

$$\epsilon^* = \epsilon^* \left(\frac{\epsilon_1}{\epsilon_2} \; , \text{ composite geometry } \right)$$

What are the effective propagation characteristics of an EM wave (radar, microwaves) in the medium?

Analytic Continuation Method for Homogenization

Bergman (1978), Milton (1979), Golden and Papanicolaou (1983), Theory of Composites, Milton (2002)

Stieltjes integral representation for homogenized parameter

separates geometry from parameters

geometry

$$F(s) = 1 - \frac{\epsilon^*}{\epsilon_2} = \int_0^1 \frac{d\mu(z)}{s - z} \qquad s = \frac{1}{1 - \epsilon_1/\epsilon_2}$$

material parameters

μ

- spectral measure of self adjoint operator $\Gamma\chi$
- mass $= p_1$
- higher moments depend on n-point correlations

$$\Gamma = \nabla(-\Delta)^{-1}\nabla\cdot$$

$\chi =$ characteristic function of the brine phase

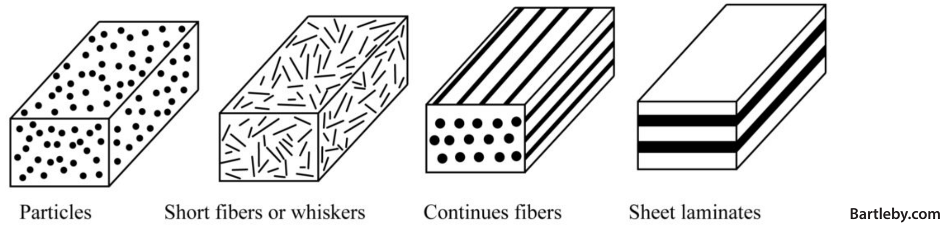
$$E = s\,(s + \Gamma\chi)^{-1} e_k$$

$\Gamma\chi$: microscale $\rightarrow$ macroscale

$\Gamma\chi$ *links scales*

Golden and Papanicolaou, Comm. Math. Phys. 1983

complexities of mixture geometry



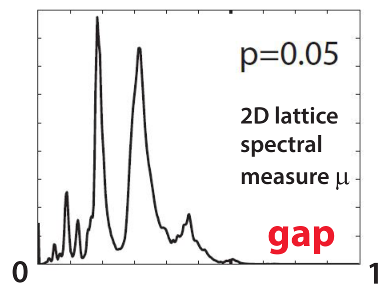
distilled

distilled

Analytic Continuation Method

Stieltjes Integral Representations
for Homogenized Parameters

Bergman 1978, Milton 1979
Golden & Papanicolaou 1983



spectral properties of operator (matrix)
~ quantum states, energy levels for atoms

eigenvectors eigenvalues

EXTEND to: polycrystals, advection diffusion, waves through ice pack

direct calculation of spectral measures

Murphy, Hohenegger, Cherkaev, Golden, *Comm. Math. Sci.* 2015

- depends only on the composite geometry
- discretization of microstructural image gives binary network
- fundamental operator becomes a random matrix
- spectral measure computed from eigenvalues and eigenvectors

once we have the spectral measure μ it can be used in Stieltjes integrals for other transport coefficients:

electrical and thermal conductivity, complex permittivity, magnetic permeability, diffusion, fluid flow properties

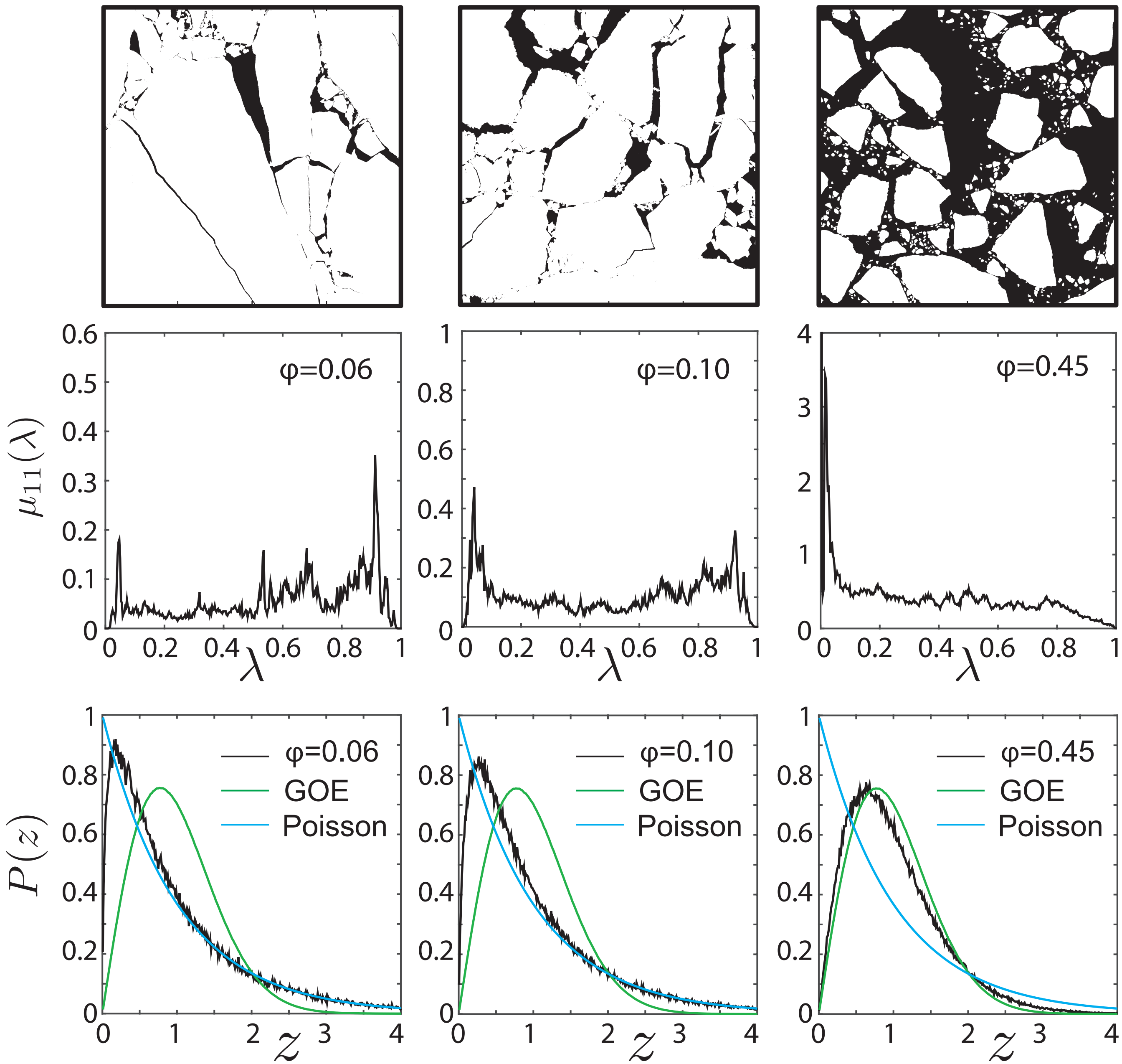
earlier studies of spectral measures

Day and Thorpe 1996
Helsing, McPhedran, Milton 2011

Spectral computations for sea ice floe configurations

spectral measures

eigenvalue spacing distributions



UNIVERSAL Wigner-Dyson distribution

uncorrelated → **level repulsion**

Eigenvalue Statistics of Random Matrix Theory

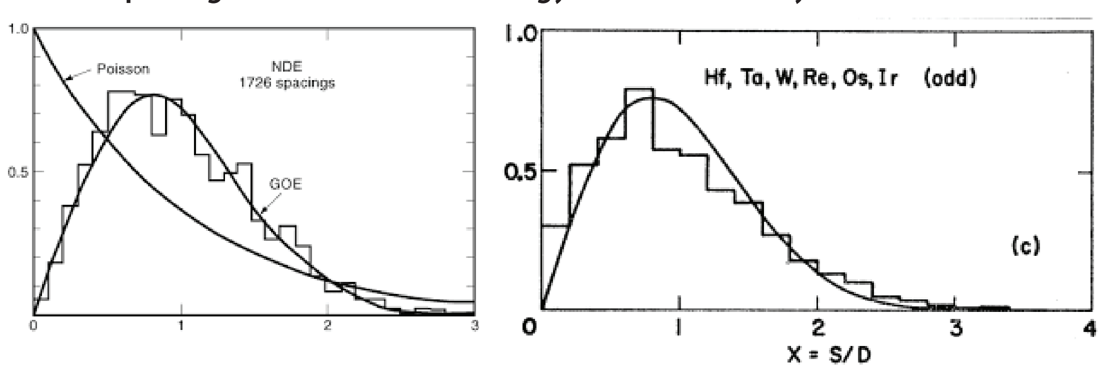
Wigner (1951) and Dyson (1953) first used random matrix theory (RMT) to describe quantized energy levels of heavy atomic nuclei.

$[\mathbf{N}]_{ij} \sim N(0,1)$, $\quad \mathbf{A} = (\mathbf{N}+\mathbf{N}^T)/2 \quad$ ***Gaussian orthogonal ensemble (GOE)***

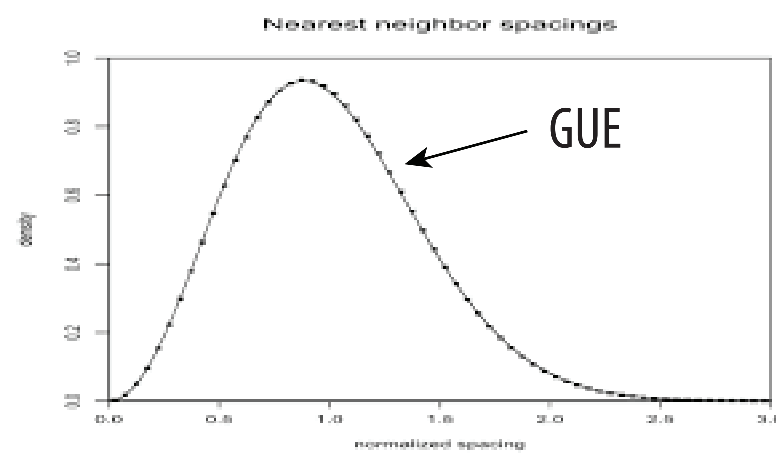
$[\mathbf{N}]_{ij} \sim N(0,1)+iN(0,1)$, $\quad \mathbf{A} = (\mathbf{N}+\mathbf{N}^\dagger)/2 \quad$ ***Gaussian unitary ensemble (GUE)***

Short range and long range correlations of eigenvalues are measured by various eigenvalue statistics.

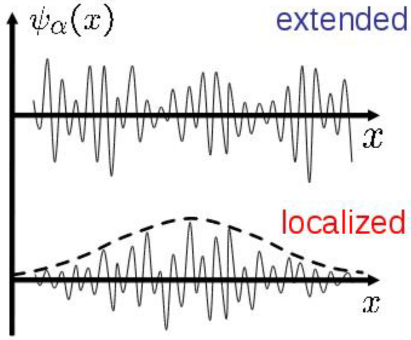
Spacing distributions of energy levels for heavy atomic nuclei



Spacing distributions of the first billion zeros of the Riemann zeta function



Universal eigenvalue statistics arise in a broad range of "unrelated" problems!



Anderson localization

disorder-driven

metal / insulator transition

Anderson 1958
Mott 1949
Evangelou 1992
Shklovshii et al 1993

propagation vs. localization in wave physics:
quantum, optics, acoustics, water waves

Wave equations

Laplace + Diffusion equations

we find percolation-driven

Anderson transition for classical transport in composites

mobility edges, localization, universal spectral statistics

Murphy, Cherkaev, Golden Phys. Rev. Lett. 2017

but no wave interference or scattering effects at play!

Where to look to see this behavior exploited in tunable media that display rich transport properties?

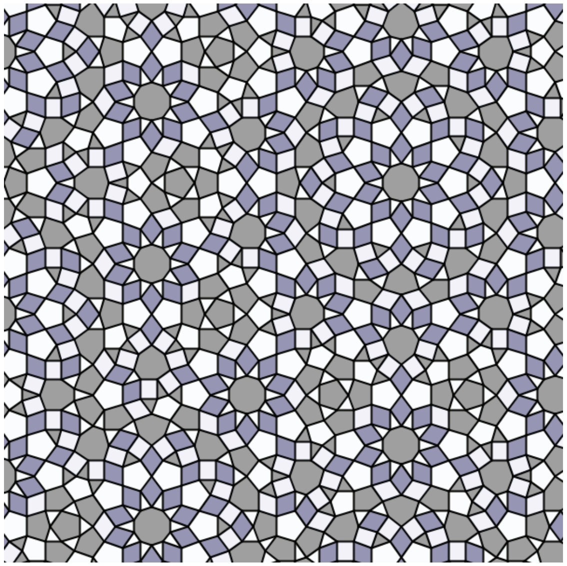
Go back to the dawn of ordered, aperiodic materials -

quasicrystals.

Shechtman et al. 1984
Levine & Steinhardt 1984

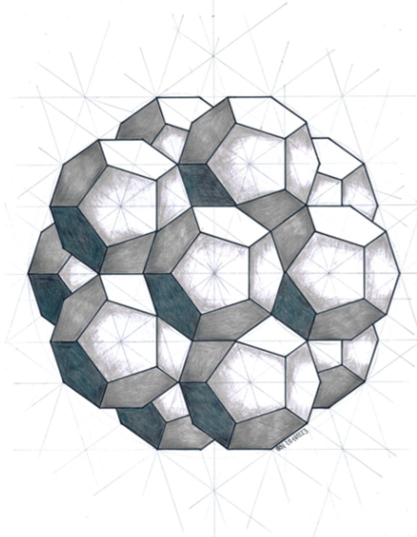
Order to Disorder in Quasiperiodic Composites

D. Morison (Physics), N. B. Murphy, E. Cherkaev, K. M. Golden, *Communications Physics* 2022



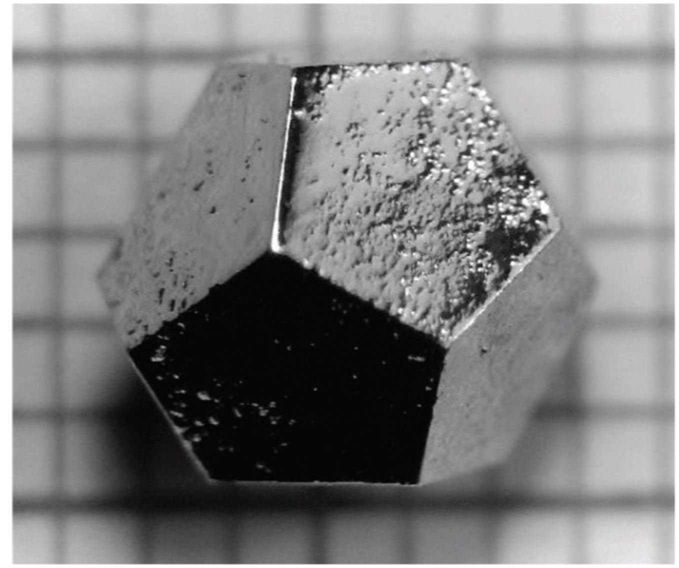
quasiperiodic checkerboard

Stampfli, 2013

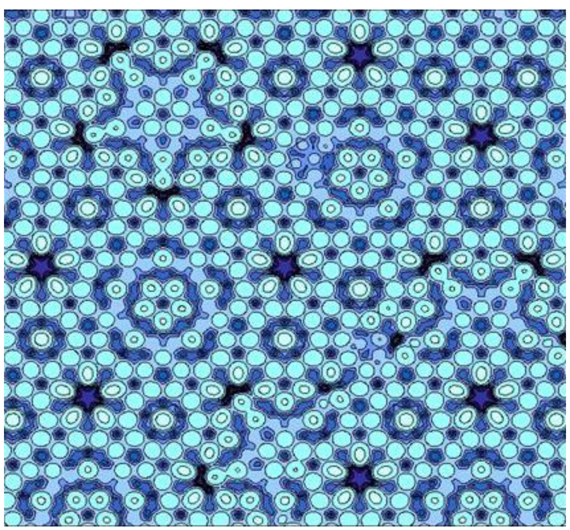


dense packing of dodecahedra

3D Penrose tiling Tripkovic, 2019



Holmium–magnesium–zinc quasicrystal



energy surface Al-Pd-Mn quasicrystal

Unal et al., 2007

quasiperiodic crystal

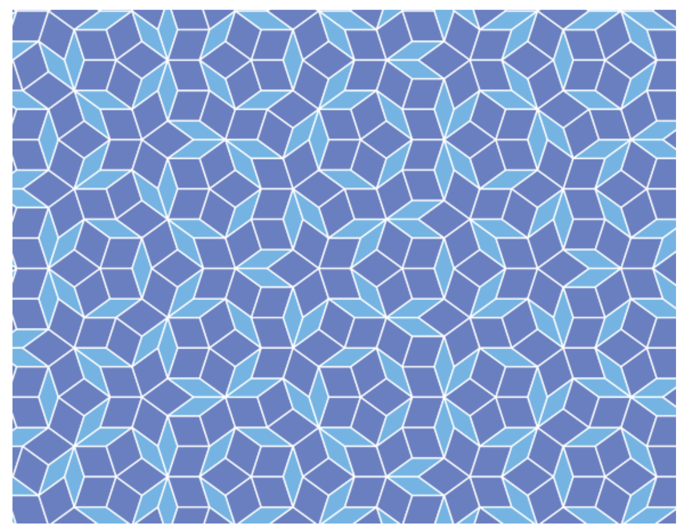
quasicrystal

ordered but aperiodic

lacks translational symmetry

Shechtman et al., 1984

Levine & Steinhardt, 1984



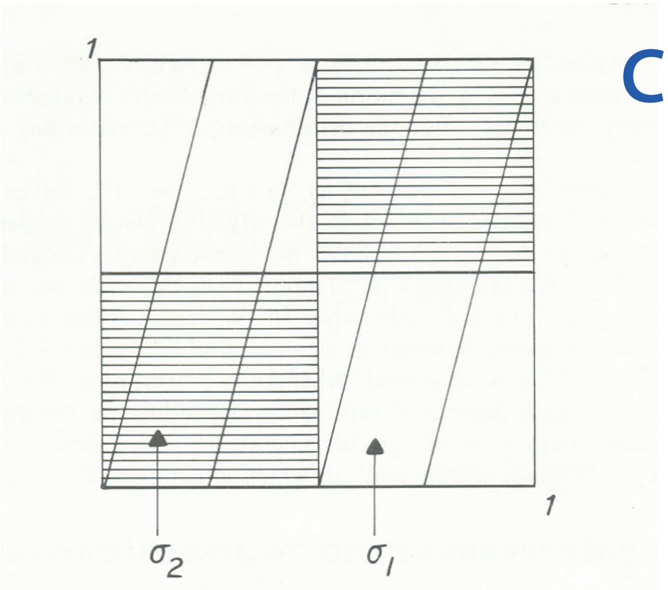
aperiodic tiling of the plane - R. Penrose 1970s local conductivity in 1D inhomogeneous material

$$\sigma(x) = 3 + \cos x + \cos kx$$

effective conductivity

$$\sigma^*(k) = \begin{cases} \text{constant} & k \;\; \text{irrational} \quad \textbf{quasiperiodic} \\ f(k) & k \;\; \text{rational} \quad \textbf{periodic} \end{cases}$$

Golden, Goldstein, Lebowitz, Phys. Rev. Lett. 1985



Classical transport in quasiperiodic media

Golden, Goldstein, and Lebowitz

***Phys. Rev. Lett.* 1985**
***J. Stat. Phys.* 1990**

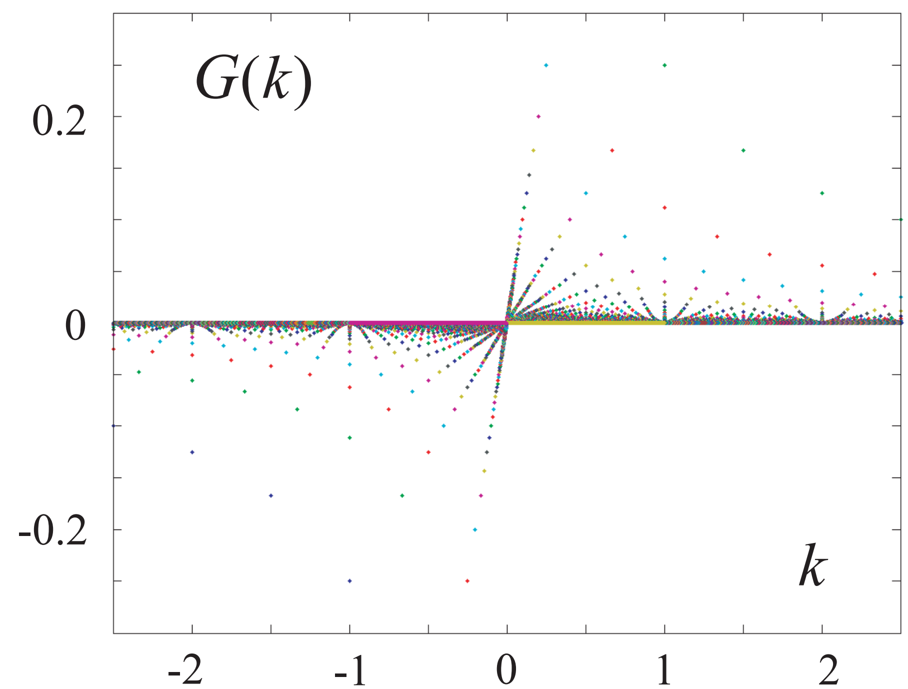
1D two component composite material

line of slope k through
an infinite checkerboard

effective conductivity $\sigma^*(k)$

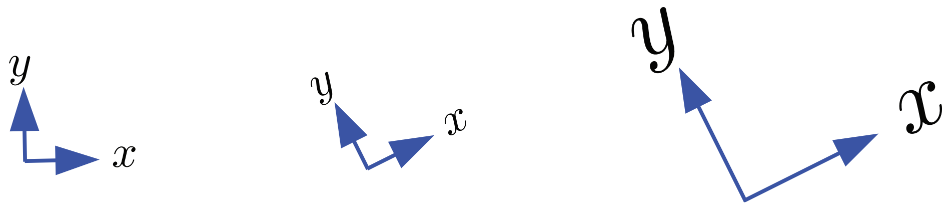
effective resistivity $1/\sigma^*(k) = 1 - G(k)$

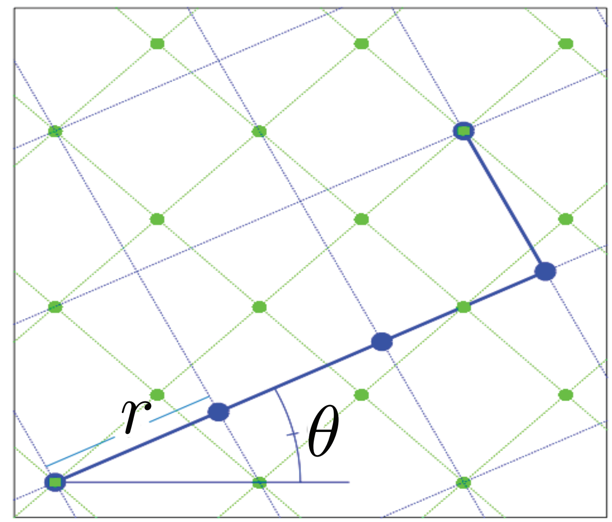
$$G(k) = \begin{cases} 0, & k \text{ irrational} \\ 1/pq, & k = p/q \text{ rational} \end{cases}$$



continuous at *k* irrational
discontinuous at *k* rational

Moiré patterns generate two component composites



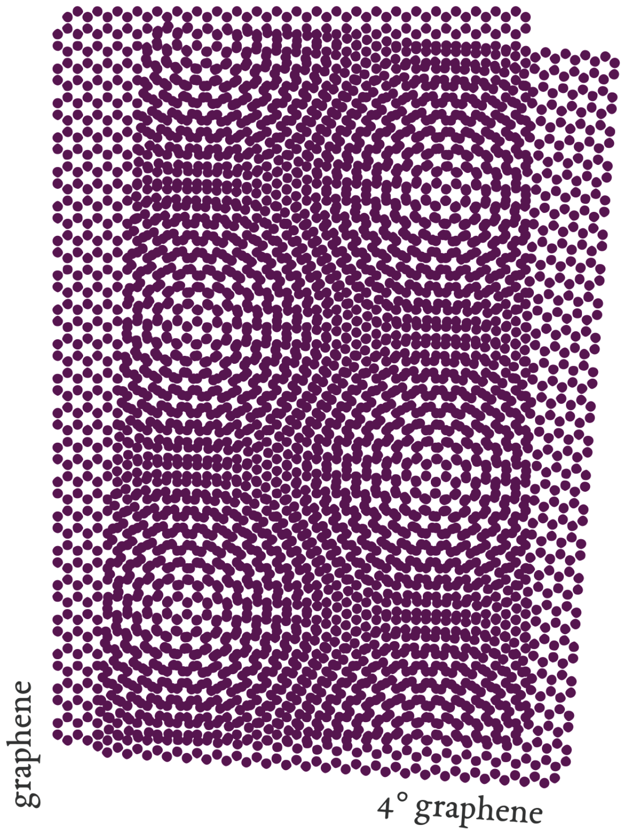


$$\begin{pmatrix} x' \\ y' \end{pmatrix} = r \begin{pmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix}$$

$$\psi\left(x', y'\right) = \cos 2\pi x' \cos 2\pi y'$$

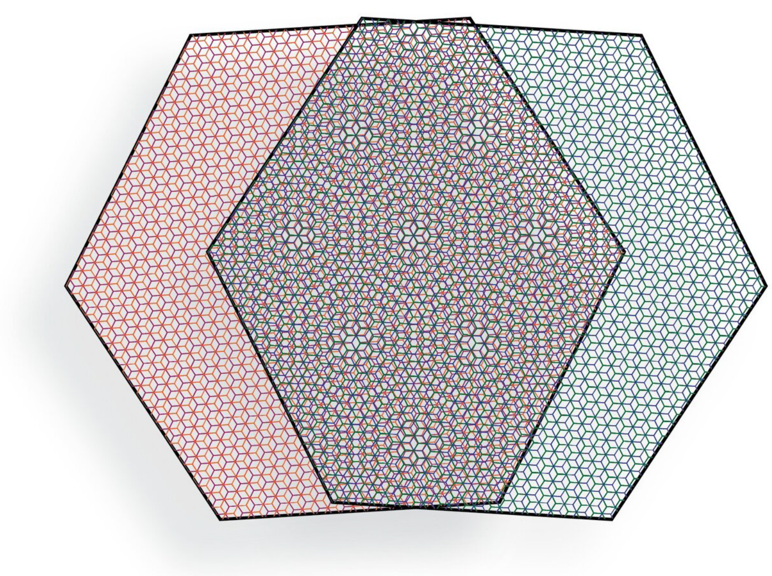
$$\chi = \begin{cases} 1, & \psi \geq 0 \\ 0, & \psi < 0 \end{cases}$$

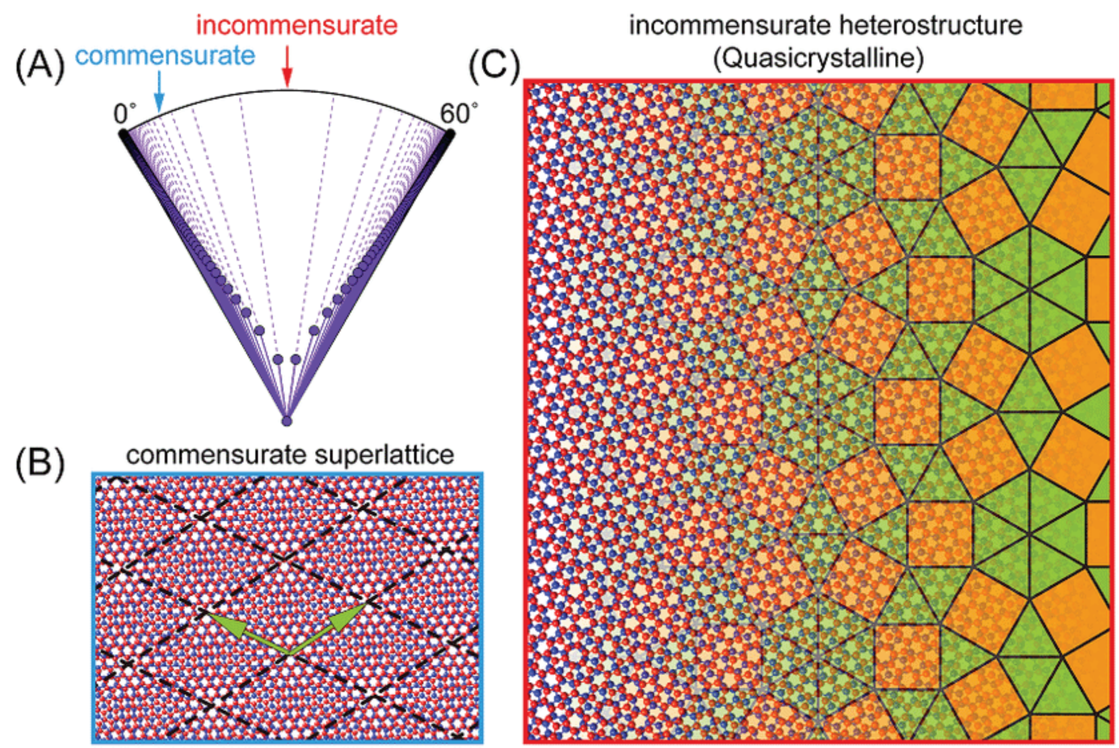
rotation and dilation



twisted bilayer graphene

superconducting
magic twist angle



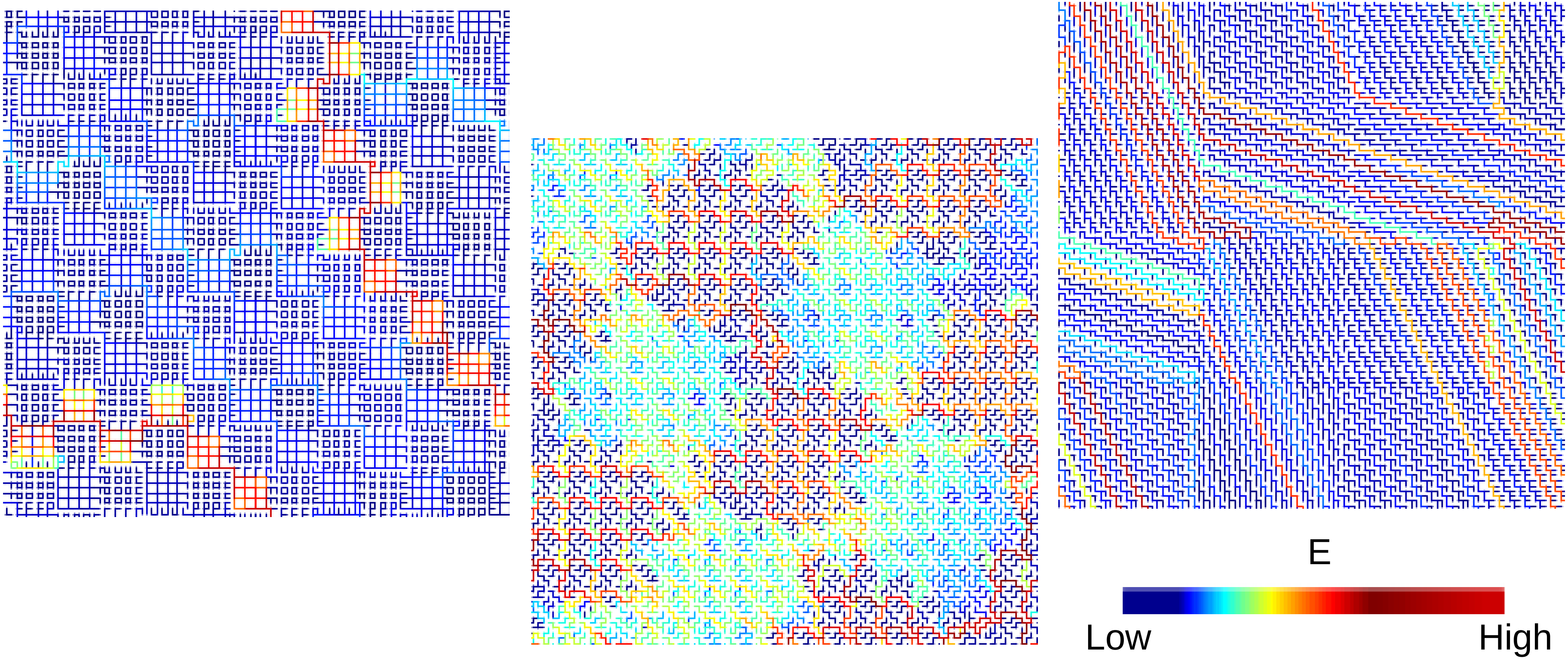


Yao et al., 2018

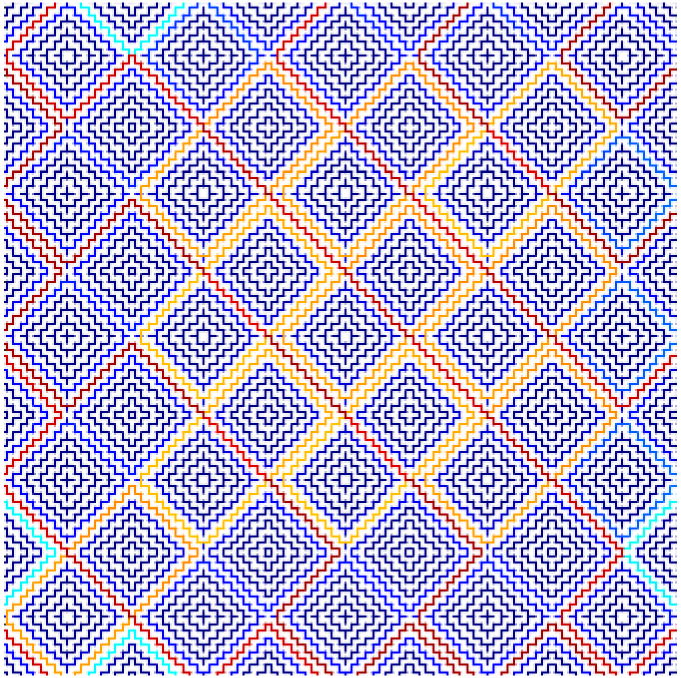
Small Difference in Moiré Parameters

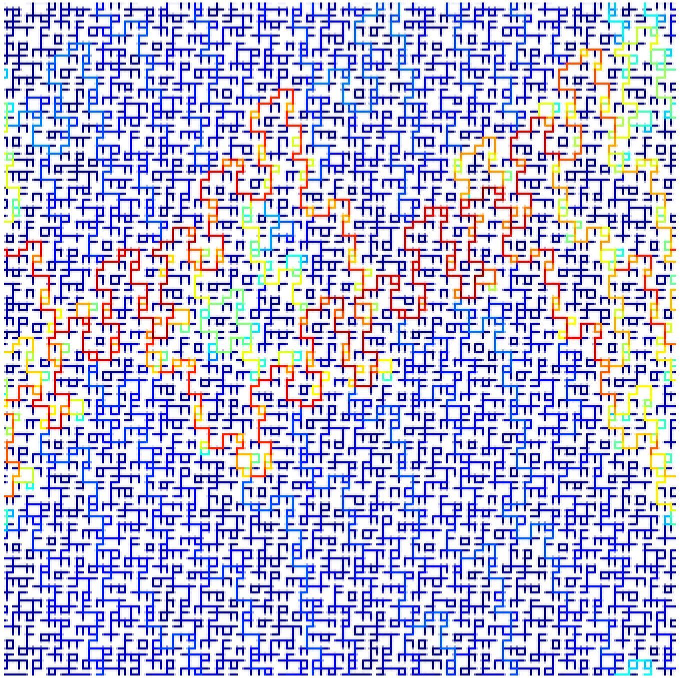
Big Difference in Material Properties

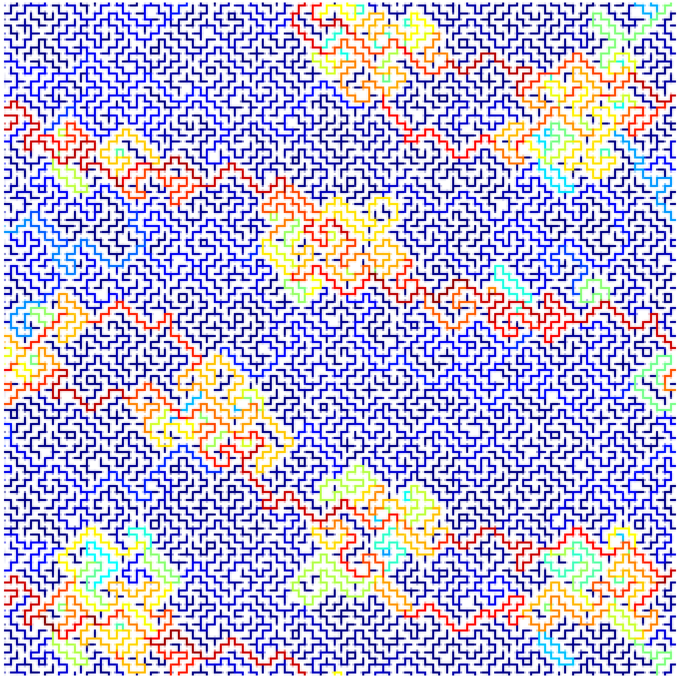
Wide Variety of Microgeometries



Wide Variety of Microgeometries







Order to disorder in quasiperiodic composites

Morison, Murphy, Cherkaev, Golden, Comm. Phys. 2022

twisted bilayer composites

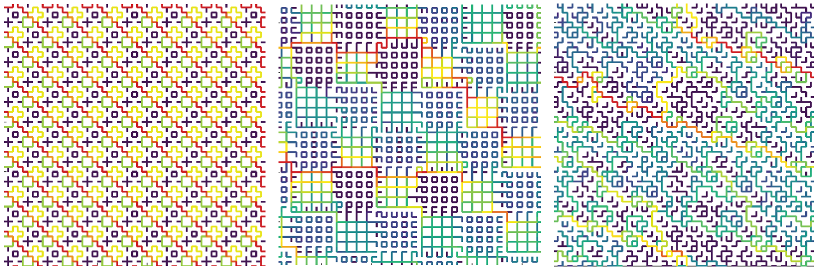
sea ice - inspired high tech spin off

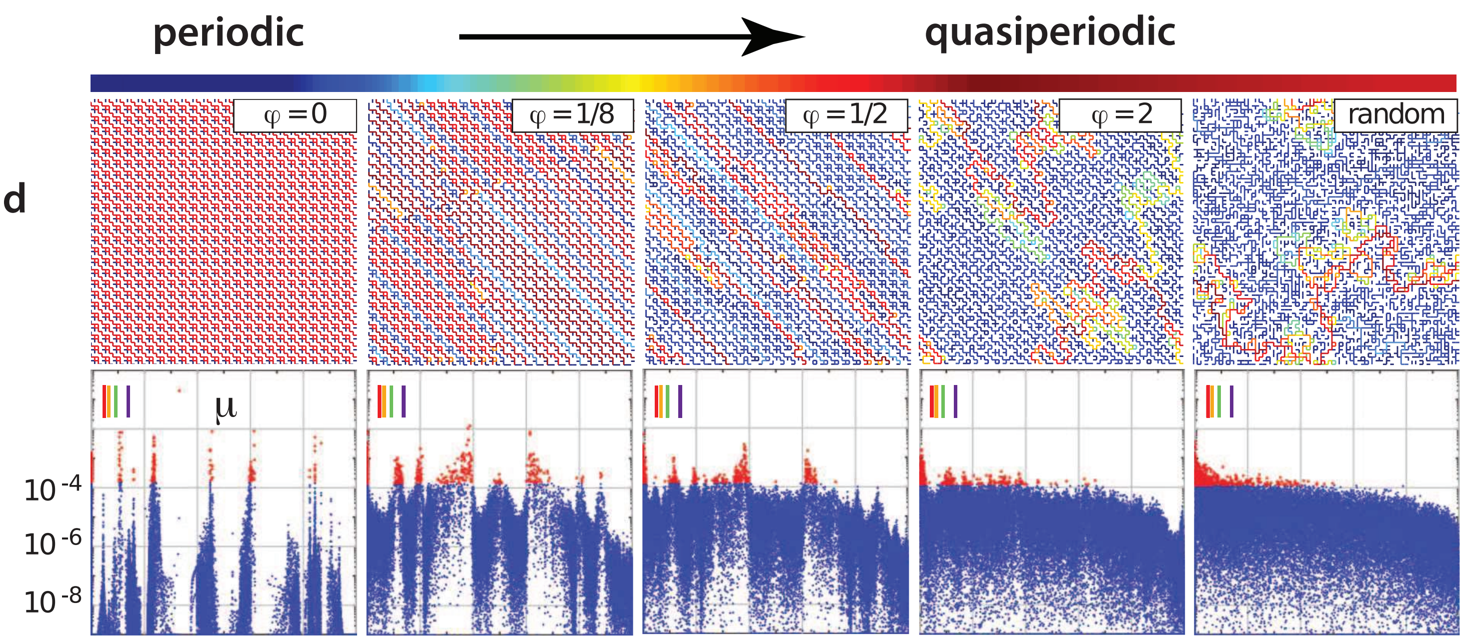
tunable Moiré composites with exotic properties

(optical, electrical, thermal, ...), Anderson localization; our Moiré patterned geometries are similar to twisted bilayer graphene

but can be engineered on any scale!

Parameterized Moiré Pattern Creates Tunable Microgeometry





electric field strength

spectral measure

RRN at percolation threshold

we bring the solid state physics framework for electronic transport and band gaps in semiconductors to classical transport in periodic and quasiperiodic composites

Anderson transition as twist angle is tuned

photonic crystals and quasicrystals

communications physics

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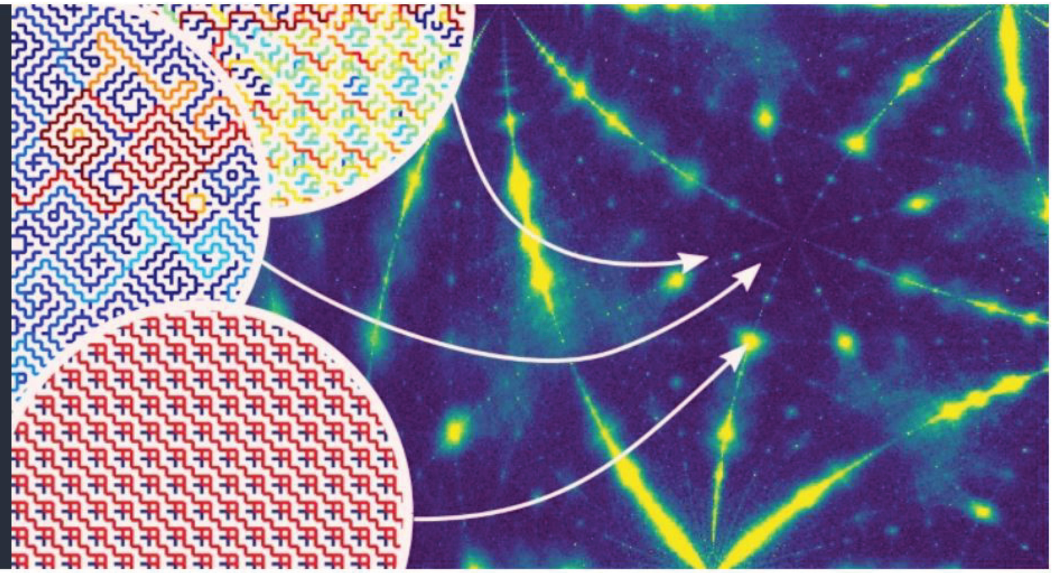
nature > communications physics

constellation of periodic systems in a sea of randomness

Order to disorder in quasiperiodic composites

David Morison, N. Benjamin Murphy ... Kenneth M. Golden

Article | 14 June 2022



Moiré parameter space

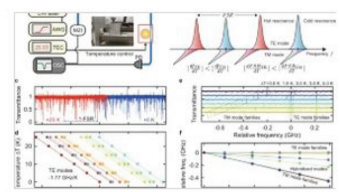
Featured

Article
Open Access
10 Jan 2023

Versatile tuning of Kerr soliton microcombs in crystalline microresonators

High-repetition rate microresonator-based frequency combs offer powerful and compact optical frequency comb sources that are of great importance to various applications. Here, the authors extend the tunability of the Kerr soliton frequency combs by exploiting thermal effects and frequency stabilization techniques.

Shun Fujii, Koshiro Wada ... Takasumi Tanabe

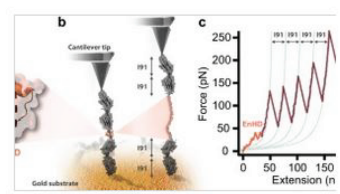


Article
Open Access
12 Jan 2023

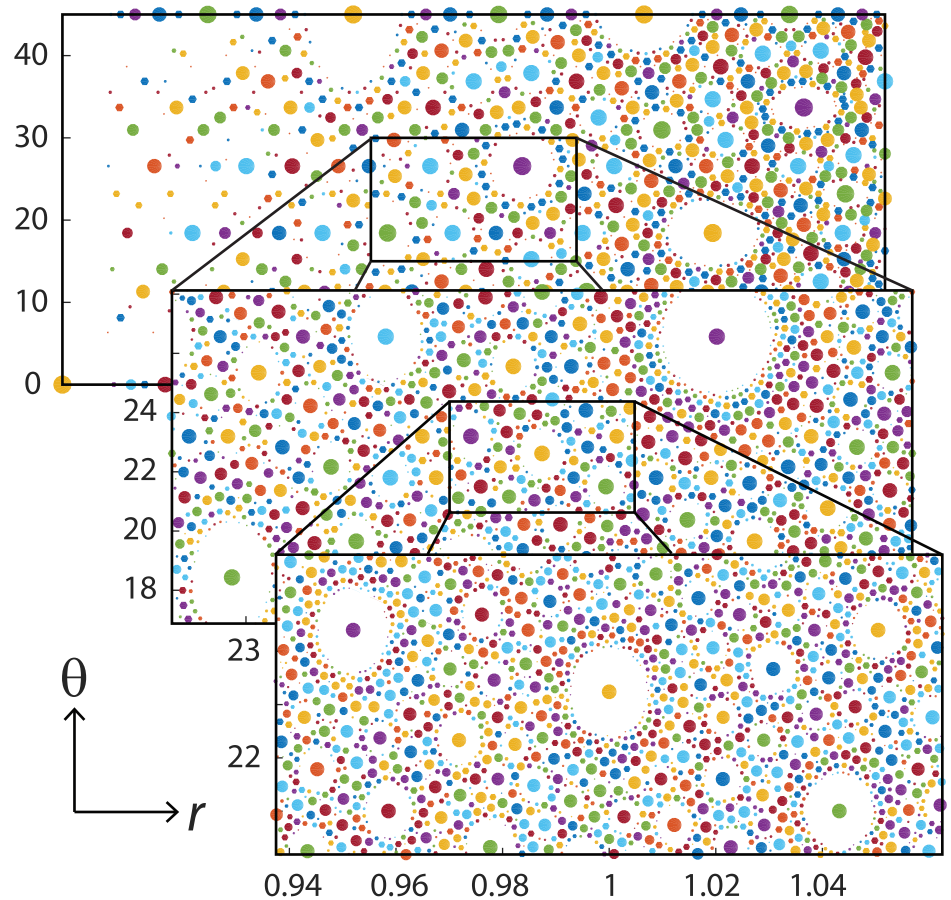
Compliant mechanical response of the ultrafast folding protein EnHD under force

Exhibiting low-energy (un)folding barriers and fast kinetics, ultrafast folding proteins are enticing models to study protein dynamics. The authors use single molecule force spectroscopy AFM to capture the compliant behaviour hallmarking the dynamics of ultrafast folding proteins under force.

Antonio Reifs, Irene Ruiz Ortiz ... Raul Perez-Jimenez



Fractal arrangement of periodic systems



Sequential insets zooming into smaller regions of parameter space.

size of the dots ~ length of period

(large dot ~ small period; small dot ~ large period; white space ~ “infinite” period)

Conclusions

1. Spectral analysis of percolation in sea ice has led to a random matrix theory picture for Anderson phenomena in classical transport through composites.

2. Here we introduce twisted bilayer composites that display exotic transport behavior as the twist angle and dilation factor are tuned.

3. Applies to all classical transport properties: electrical and thermal conductivity, optical, diffusive, etc. -- OVER ALL LENGTH SCALES

Modeling sea ice leads to unexpected areas of math, physics, and engineering!

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Notices

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AMS AMERICAN MATHEMATICAL SOCIETY
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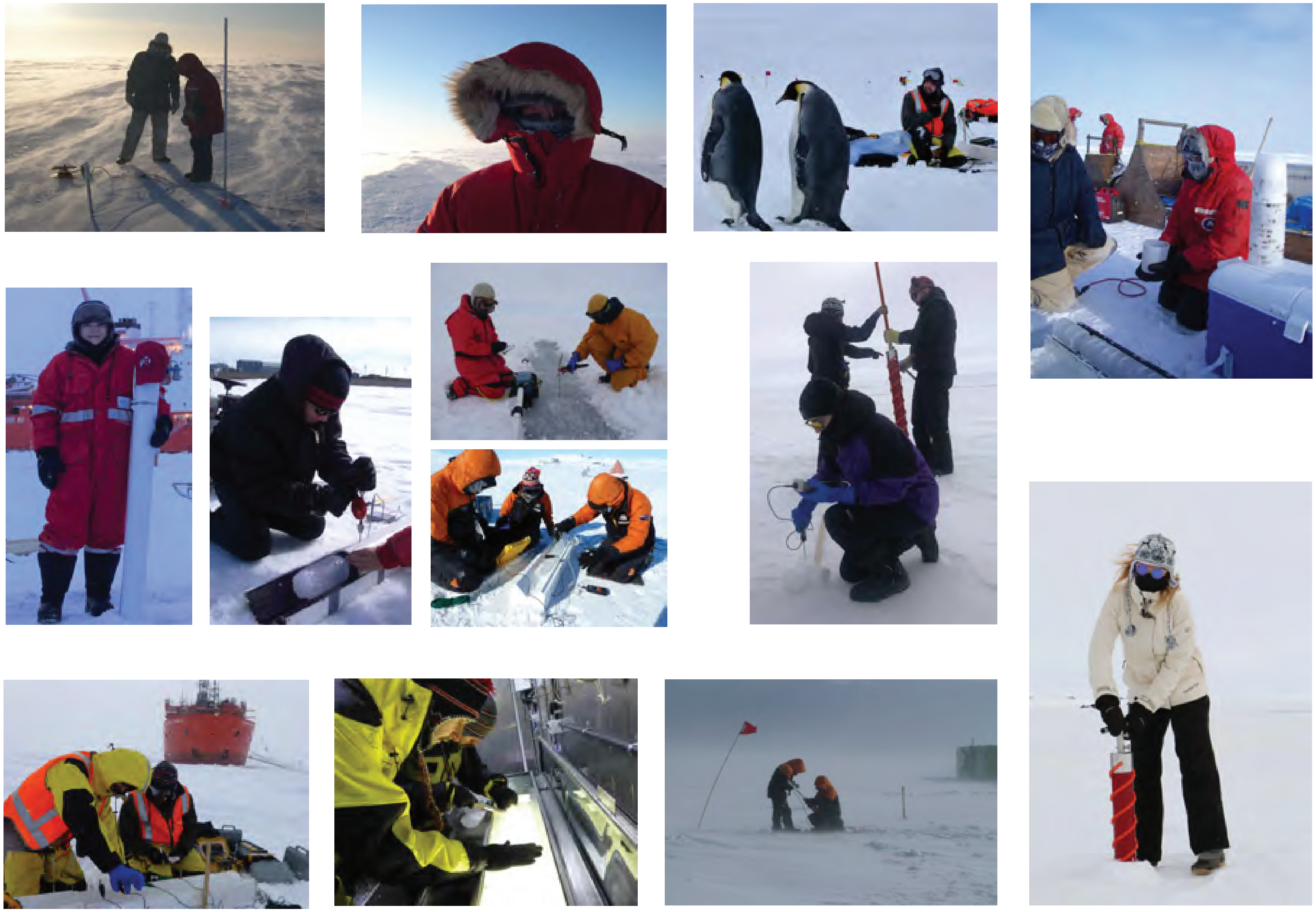
The cover is based on “Modeling Sea Ice,” page 1535.

Thank you to so many postdocs, graduate students, undergraduates, high school students and colleagues who contributed to this work!



U. of Utah students in the Arctic and Antarctic (2003-2022): closing the gap between theory and observation - making math models come alive and experiencing climate change firsthand.

THANK YOU

Office of Naval Research

Applied and Computational Analysis Program

Arctic and Global Prediction Program

National Science Foundation

Division of Mathematical Sciences

Division of Polar Programs

United States Coast Guard · Semper Paratus · 1790

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